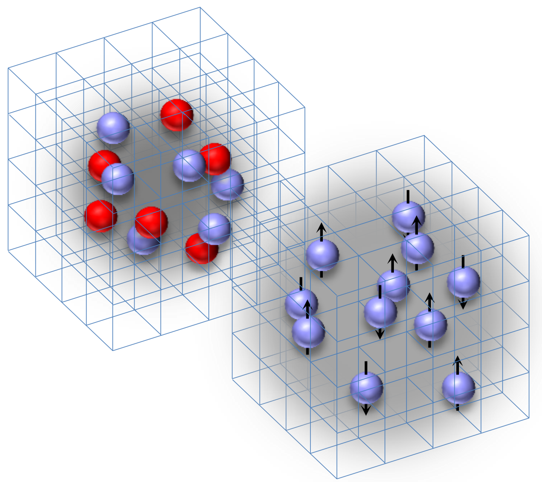
Lattice Simulations: ^{16}O Structure and New Methods



Nuclear Lattice EFT Collaboration

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TRIUMF
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Outline

What is lattice effective field theory?

Overview of methods

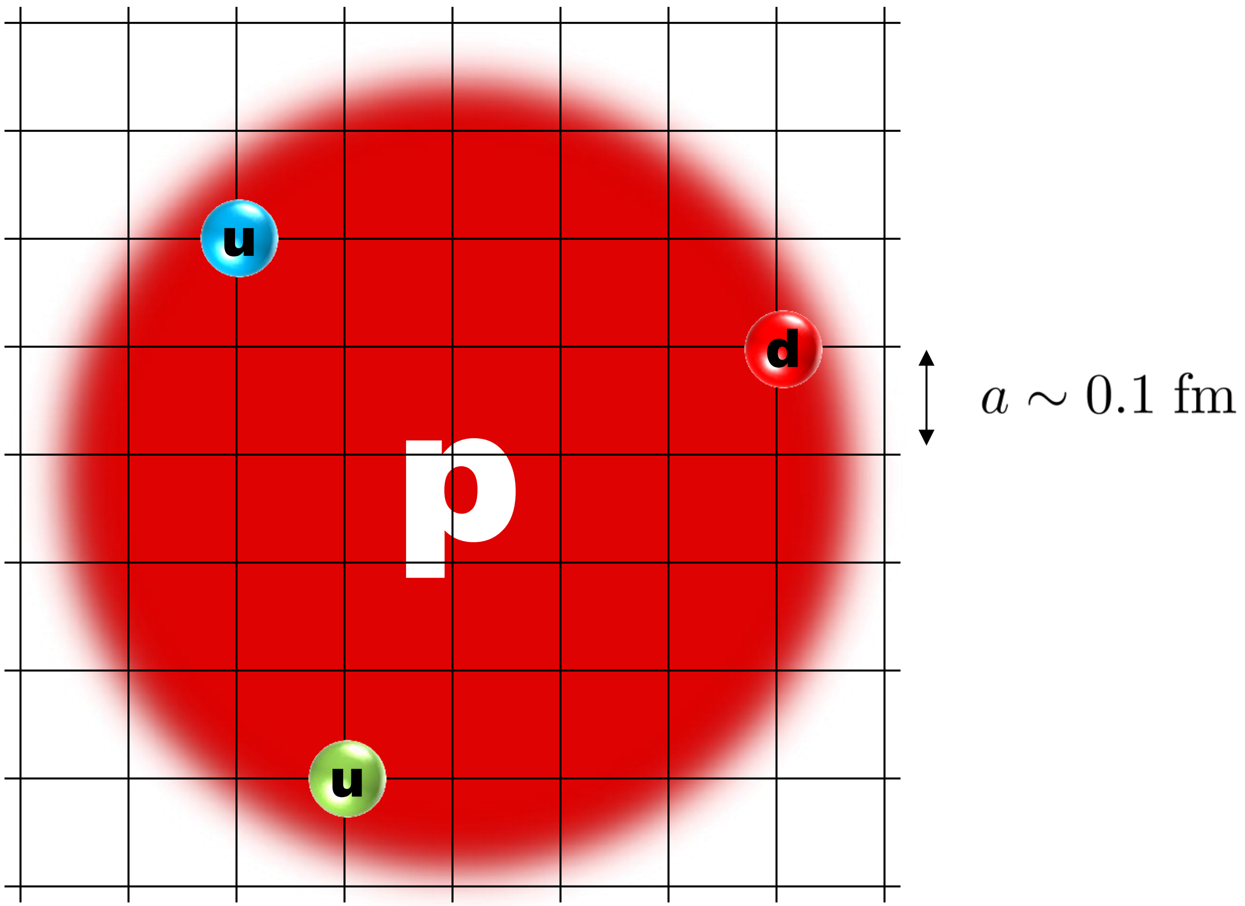
Oxygen-16 structure and spectrum

Symmetry Sign Interpolation Method

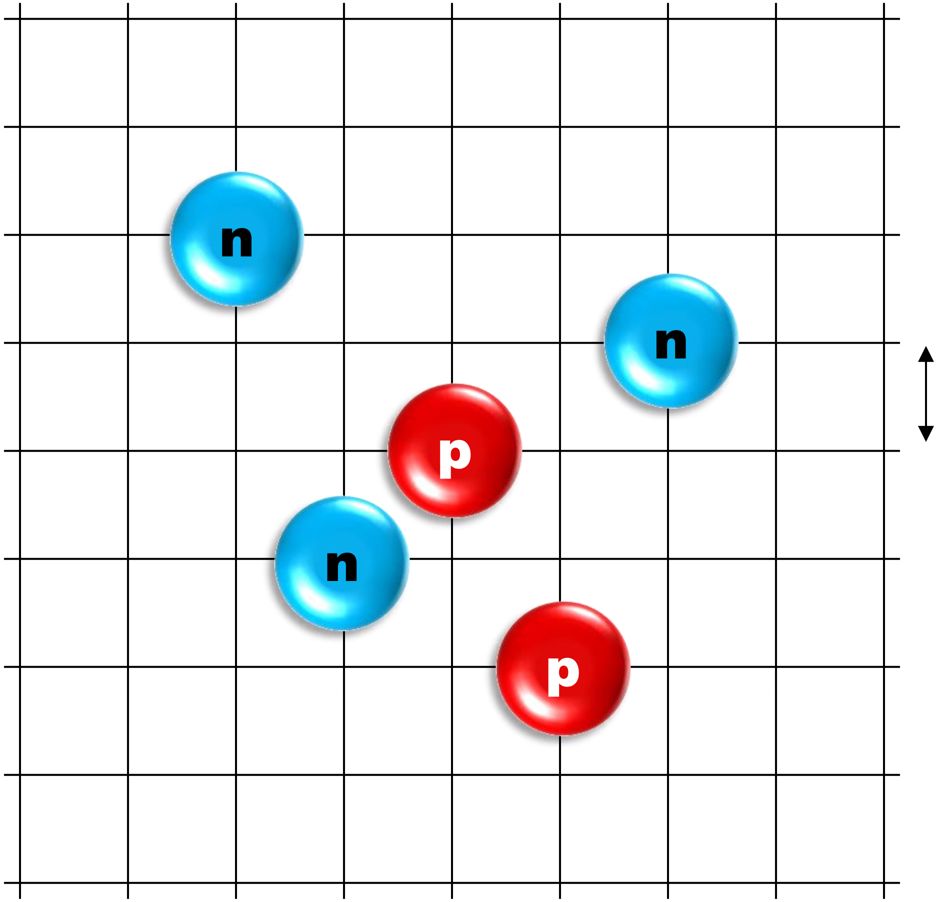
Beryllium-10 ground state

Summary and future directions

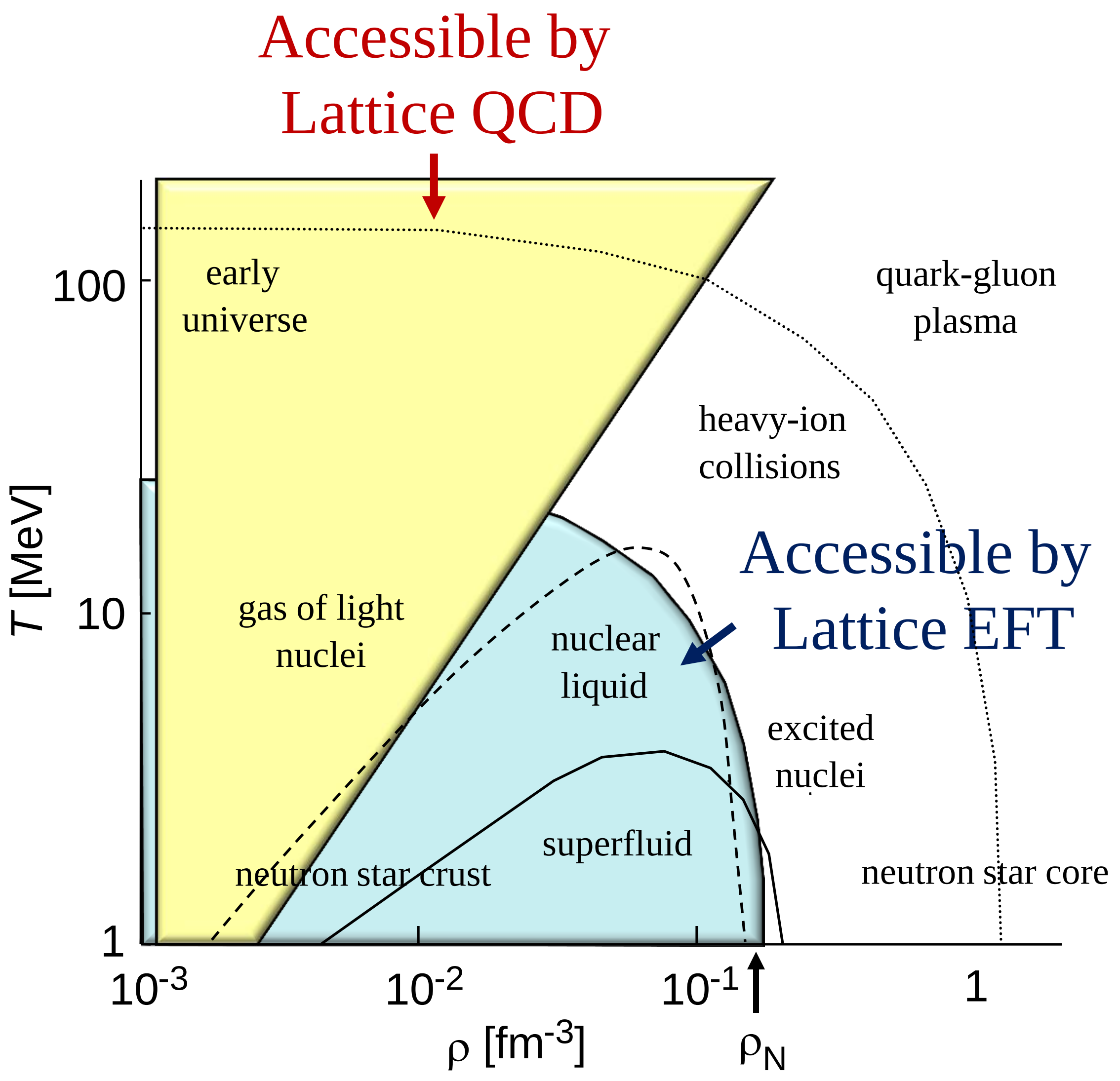
Lattice quantum chromodynamics



Lattice effective field theory

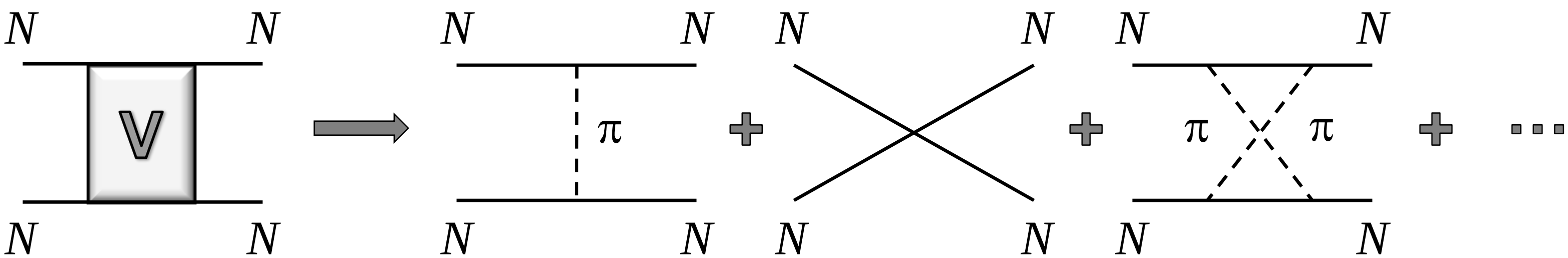


$a \sim 1 - 5$ fm


Accessible by
Lattice QCD
early
universe
quark-gluon
plasma
heavy-ion
collisions
Accessible by
Lattice EFT
gas of light
nuclei
nuclear
liquid
excited
nuclei
superfluid
neutron star crust
neutron star core
100
10
1
T [MeV]
10^{-3}
10^{-2}
10^{-1}
1
ρ [fm^{-3}]
ρ_N

Low energy nucleons: Chiral effective field theory

Construct the effective potential order by order



V^{OPEP} Contact interactions V^{TPEP}

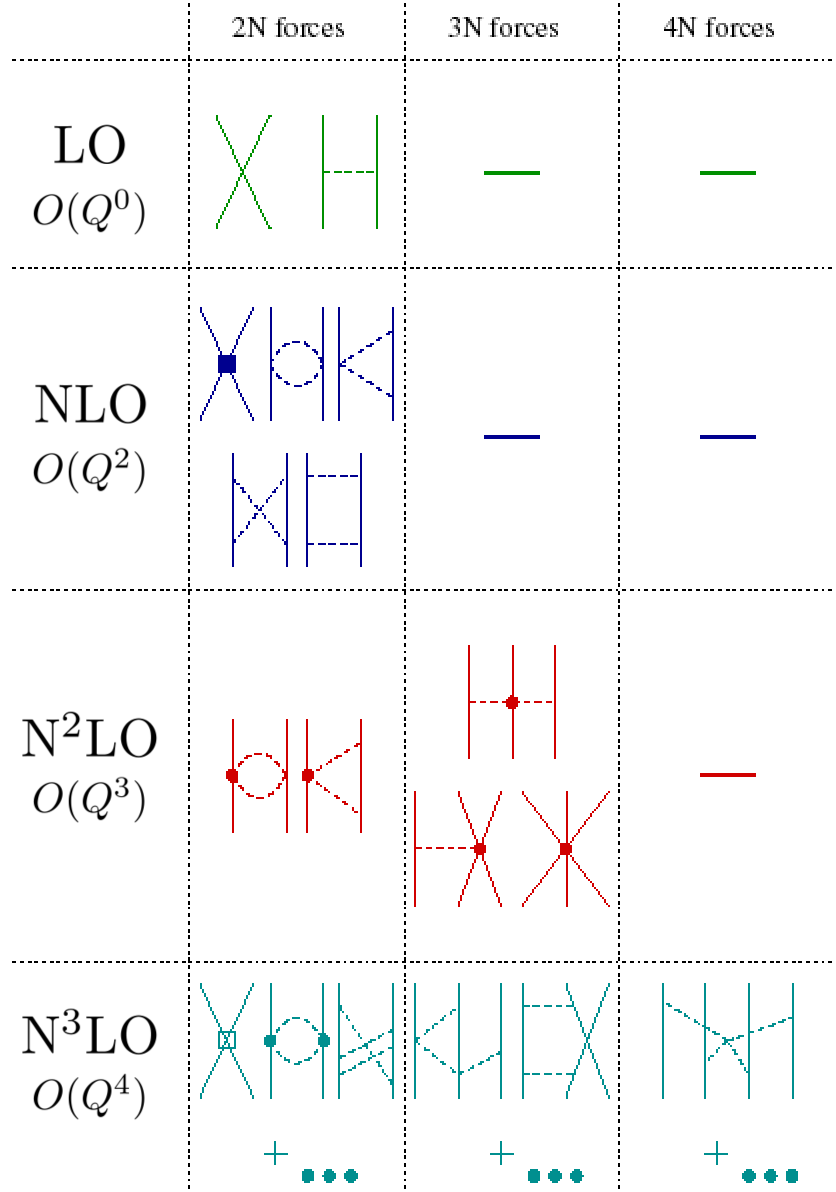
Leading order (LO) Next-to-leading order (NLO)

Nuclear Scattering Data

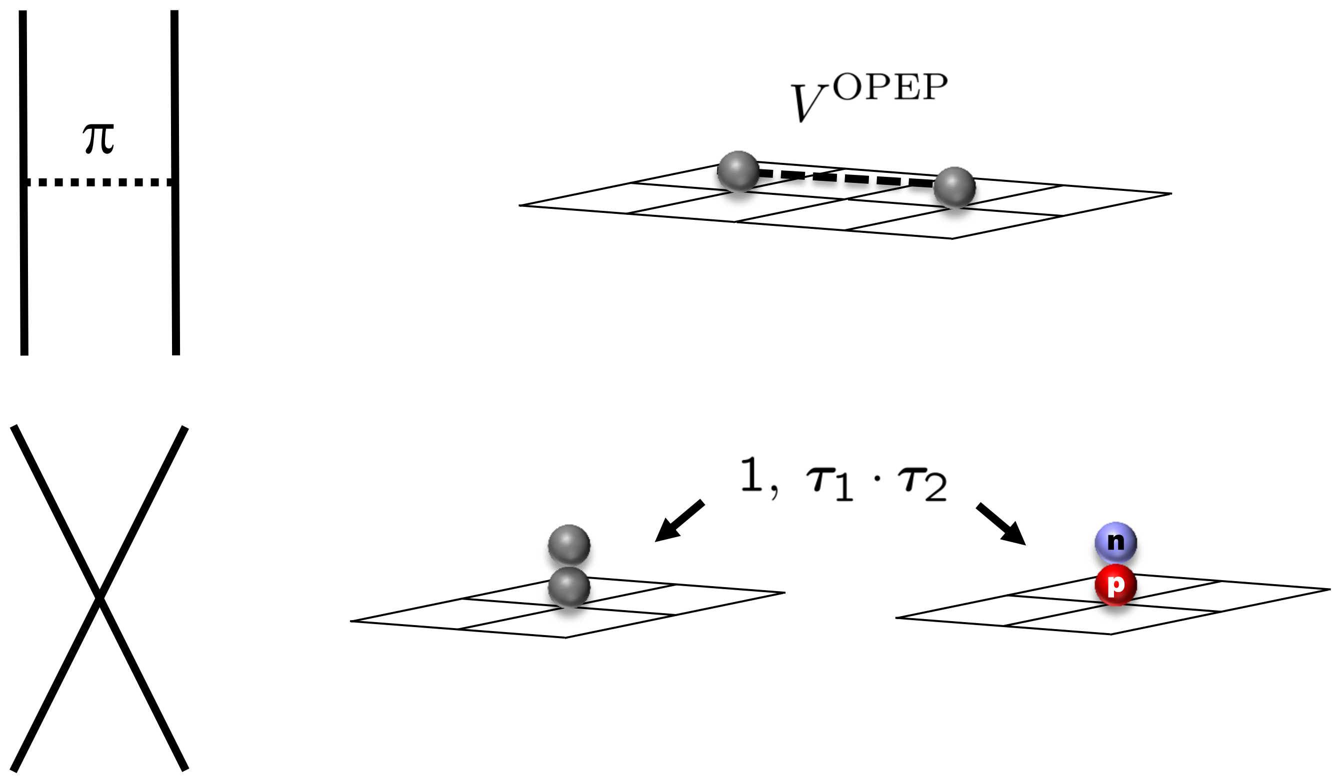
↓

Effective Field Theory

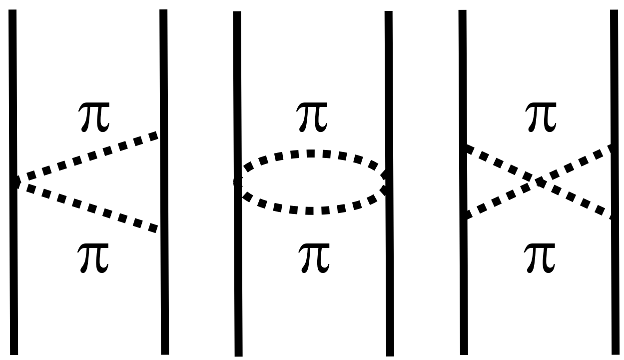
Ordonez et al. '94; Friar & Coon '94; Kaiser et al. '97; Epelbaum et al. '98,'03; Kaiser '99-'01; Higa et al. '03; …



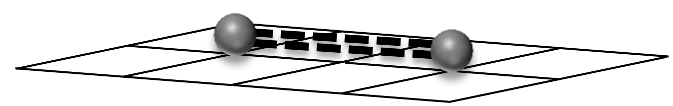
Leading order on the lattice

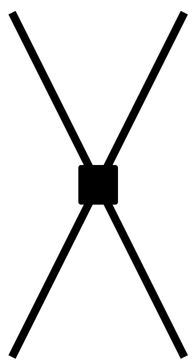


Next-to-leading order on the lattice

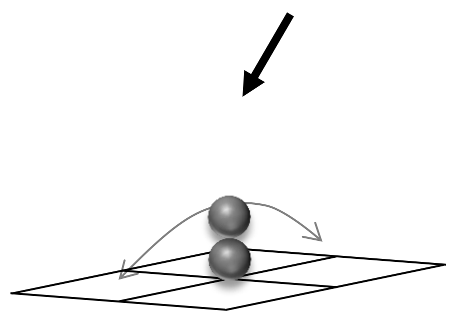


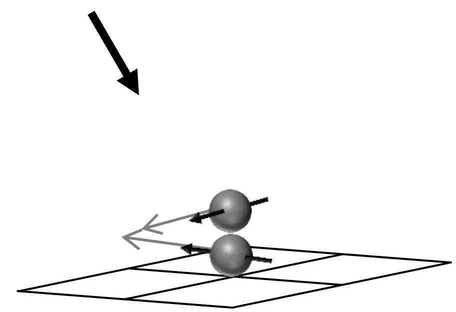
V^{TPEP}





$\vec{\nabla}_1 \cdot \vec{\nabla}_2 \qquad (\vec{\sigma}_1 \cdot \vec{\nabla}_1)\,(\vec{\sigma}_2 \cdot \vec{\nabla}_2) \qquad \cdots$



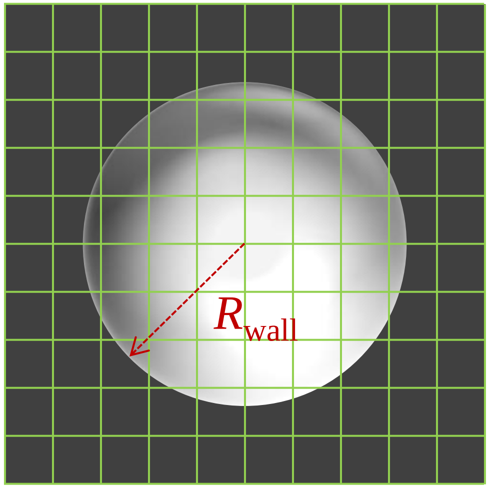


Physical scattering data → Unknown operator coefficients

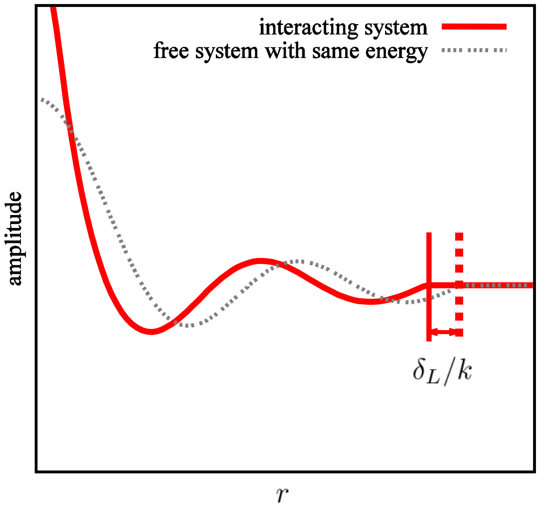
Spherical wall method

Borasoy, Epelbaum, Krebs, D.L., Meißner, EPJA 34 (2007) 185

Spherical wall imposed in the center of mass frame

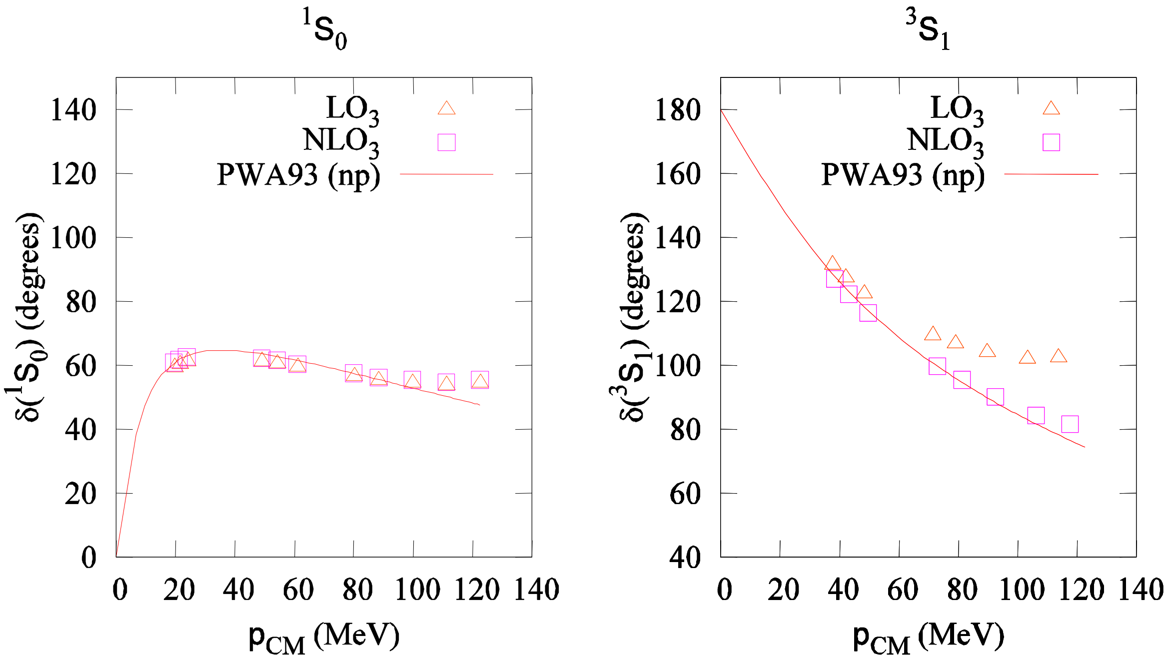


Representation	J_z	Example
A_1	$0 \bmod 4$	$Y_{0,0}$
T_1	$0,1,3 \bmod 4$	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	$0,2 \bmod 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$
T_2	$1,2,3 \bmod 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$
A_2	$2 \bmod 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$



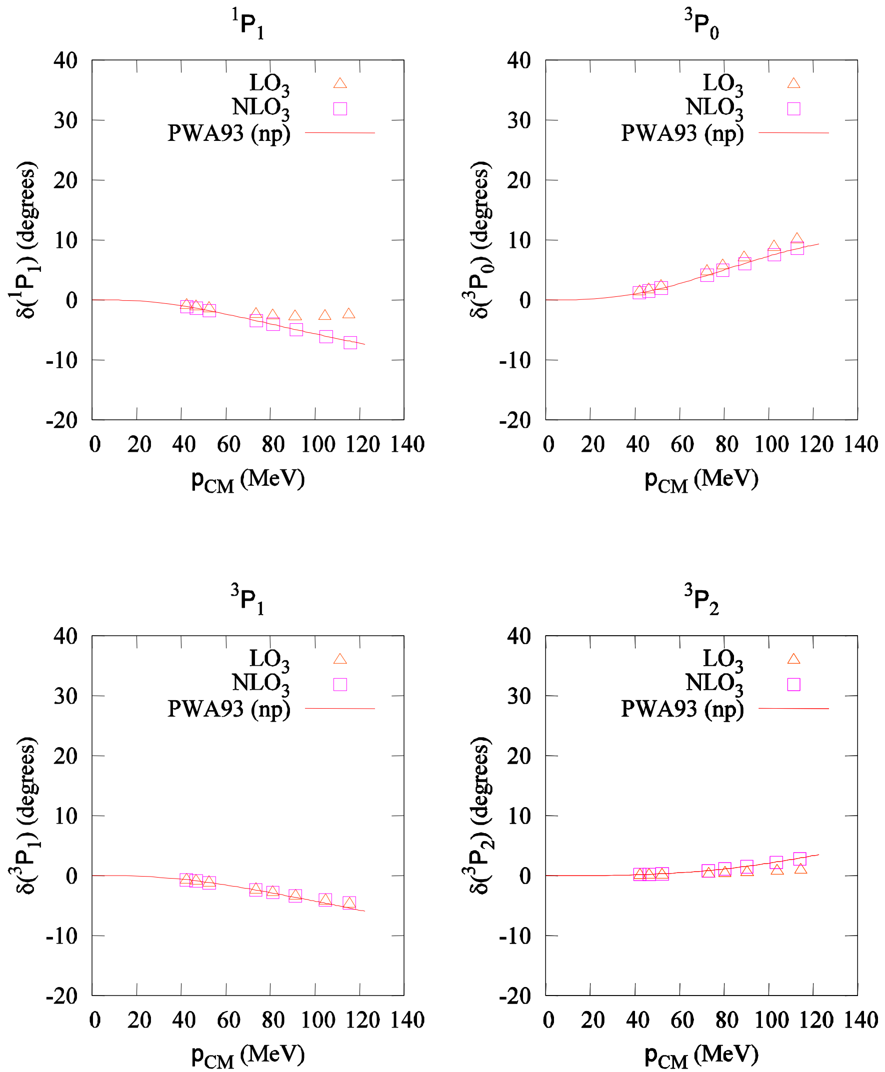
LO_3: S waves

$a = 1.97$ fm

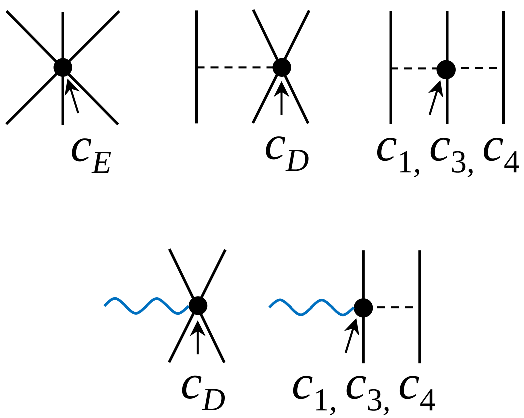


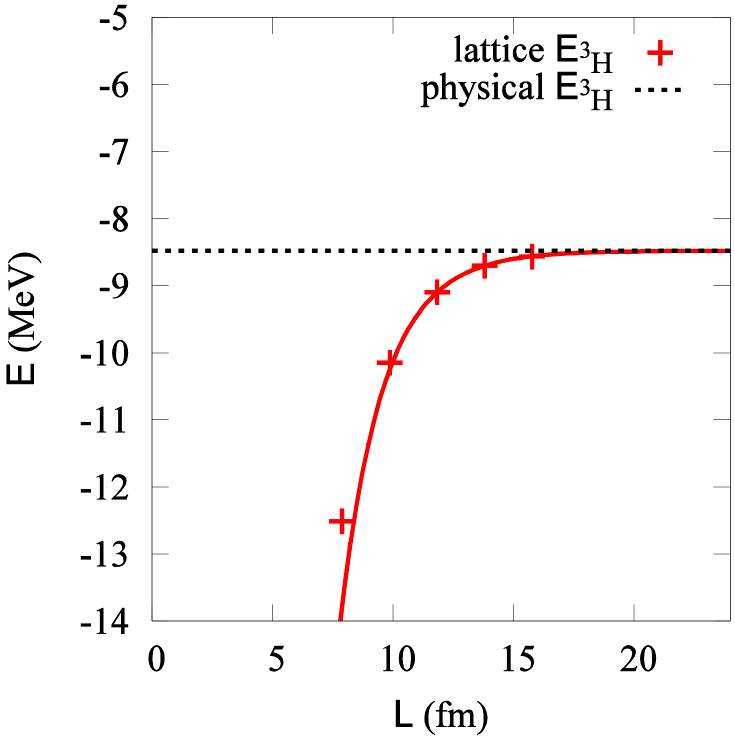
LO$_3$: P waves

$a = 1.97$ fm



Two unknown coefficients at NNLO from three-nucleon forces.
Determine c_D and c_E using ^{3}H binding energy and the weak axial current at low cutoff momentum.



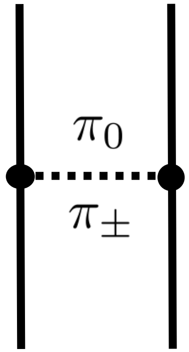


Park, et al., PRC 67 (2003) 055206,
Gårdestig, Phillips, PRL 96 (2006) 232301,
Gazit, Quaglioni, Navratil, PRL 103 (2009) 102502

Neutrons and protons: Isospin breaking and Coulomb

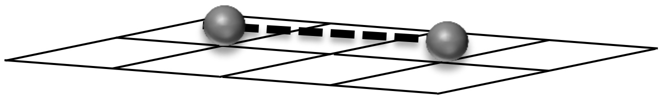
Isospin-breaking and power counting *[Friar , van Kolck, PRC 60 (1999) 034006; Walzl, Meißner, Epelbaum NPA 693 (2001) 663; Friar, van Kolck, Payne, Coon, PRC 68 (2003) 024003; Epelbaum, Meißner, PRC72 (2005) 044001…]*

Pion mass difference

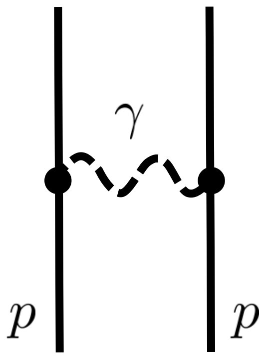


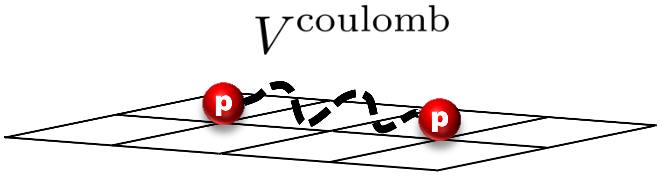
$$m_{\pi_0} \neq m_{\pi_\pm}$$

$$V_{\pi_0}^{\mathrm{OPEP}}, V_{\pi_\pm}^{\mathrm{OPEP}}$$

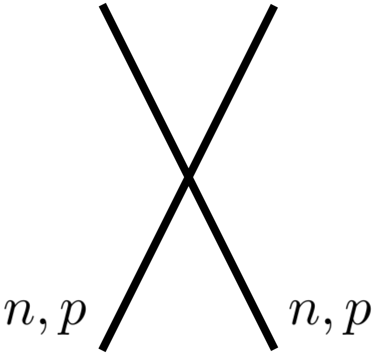


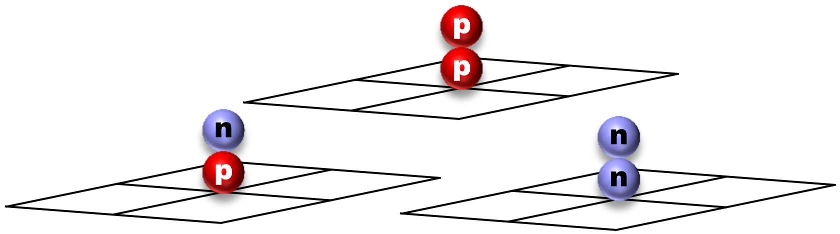
Coulomb potential



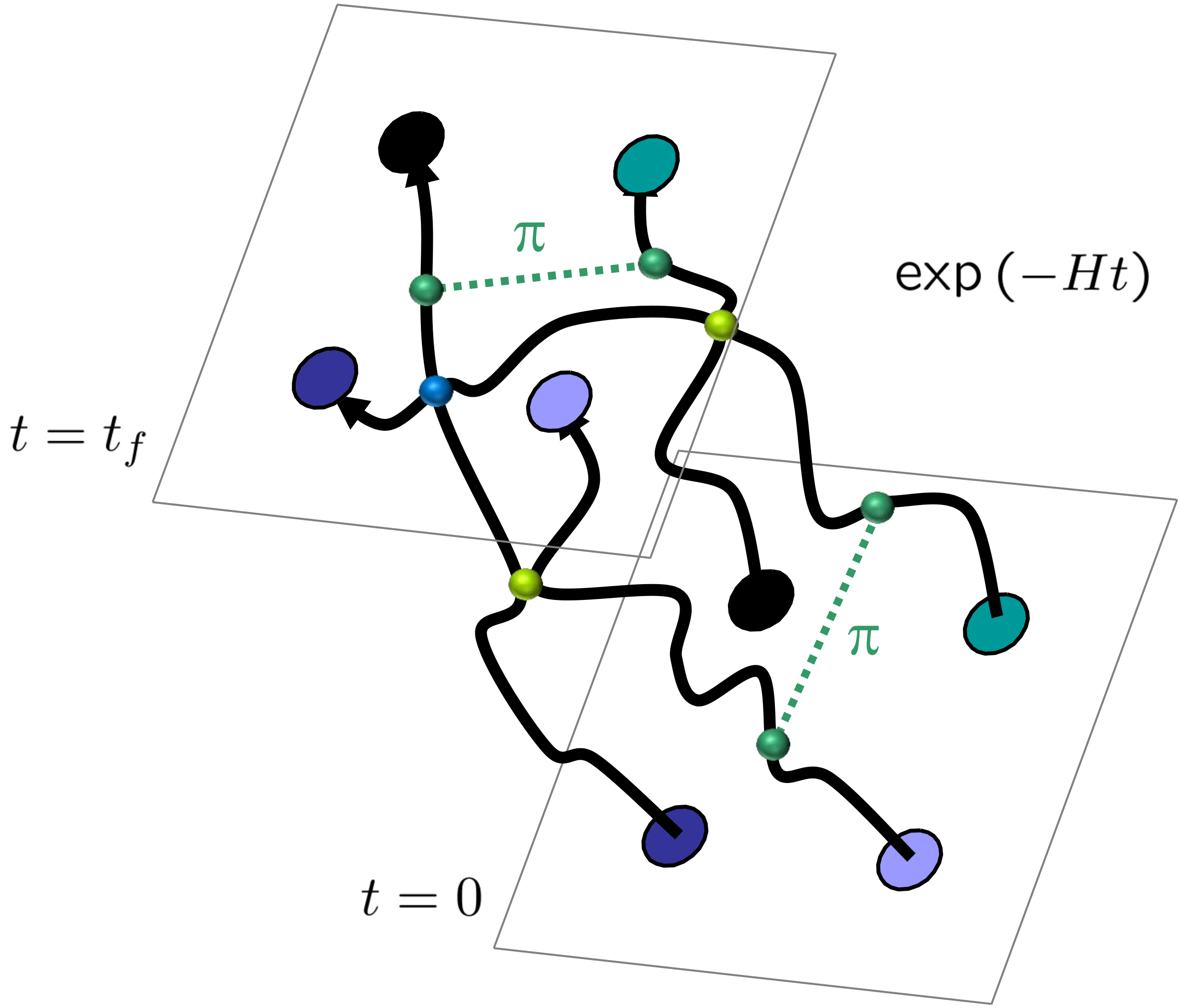


Charge symmetry breaking
Charge independence breaking





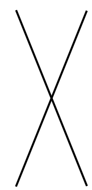
Euclidean time projection



Auxiliary field method

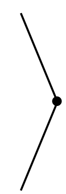
We can write exponentials of the interaction using a Gaussian integral identity

$$\exp\left[-\frac{C}{2}(N^{\dagger}N)^{2}\right]$$



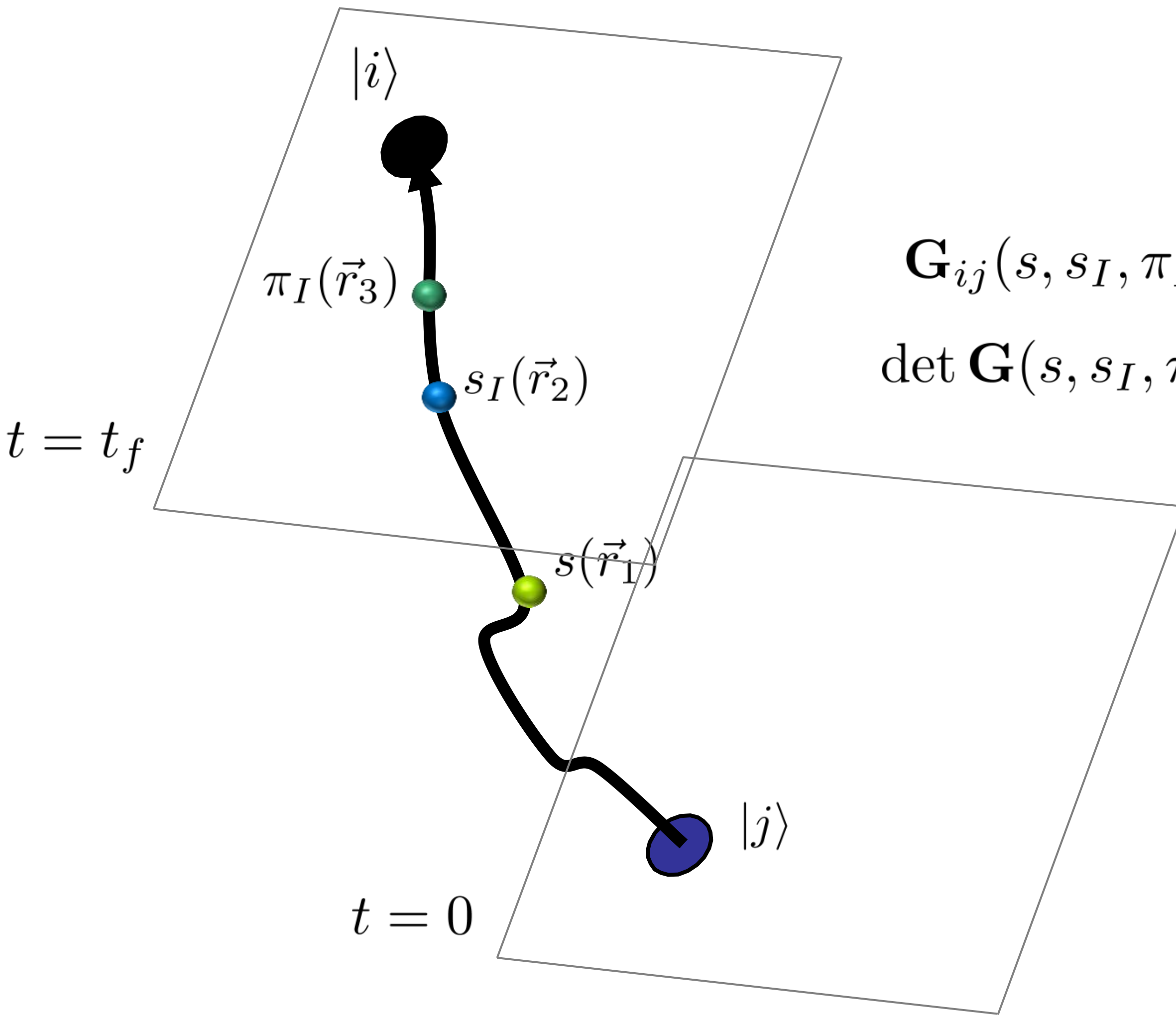
$$(N^{\dagger}N)^{2}$$

$$= \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^{2}+\sqrt{-C}\, s(N^{\dagger}N)\right]$$



$$sN^{\dagger}N$$

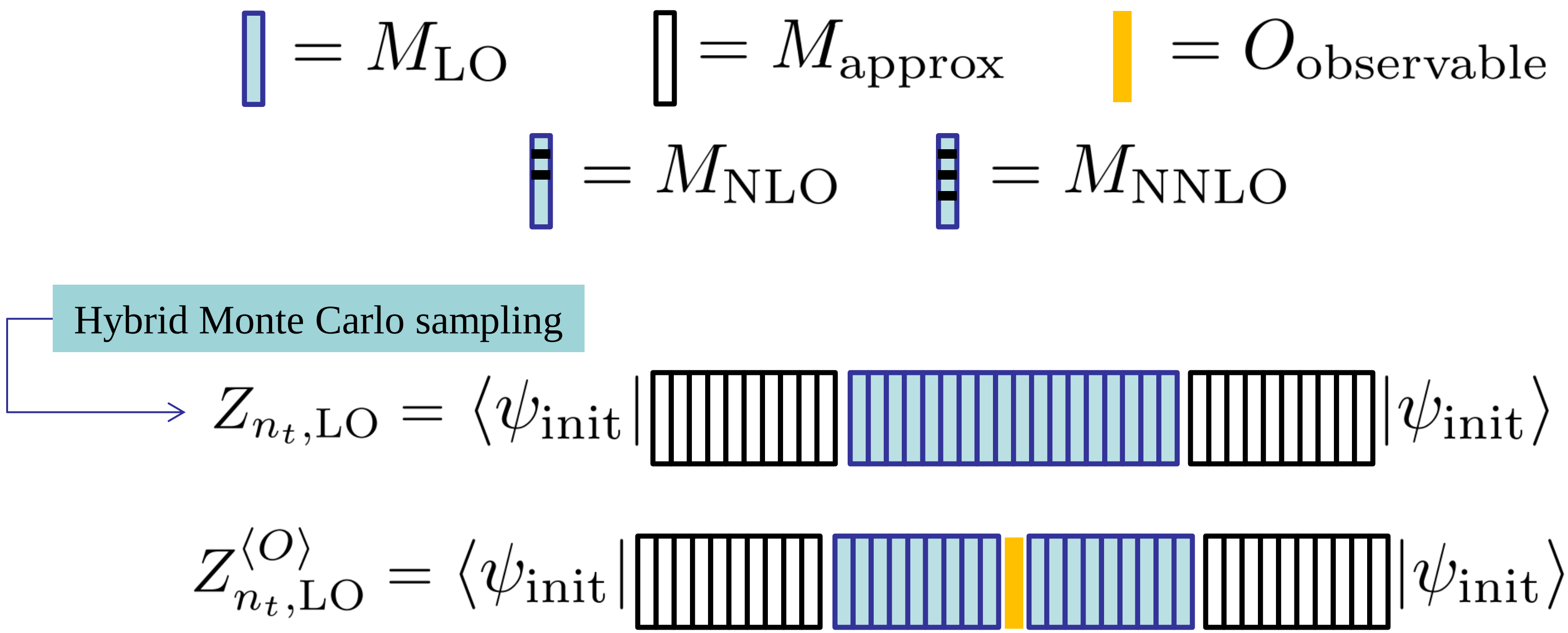
We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.



$\mathbf{G}_{ij}(s, s_I, \pi_I)$

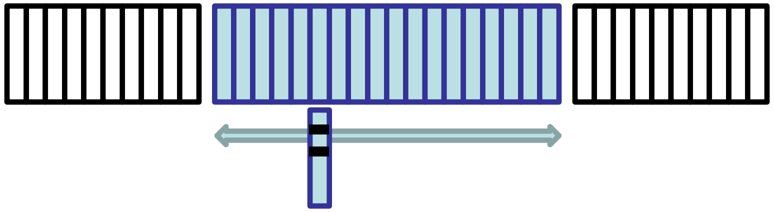
$\det \mathbf{G}(s, s_I, \pi_I)$

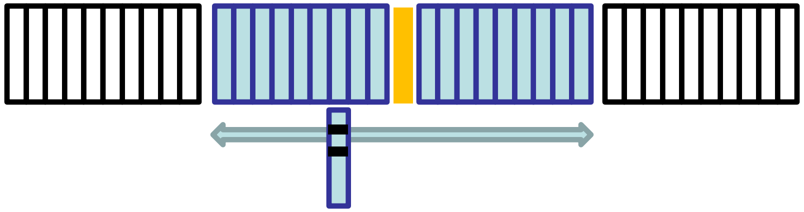
Schematic of lattice Monte Carlo calculation



$$e^{-E_{0,\text{LO}}a_t} = \lim_{n_t\to\infty} Z_{n_t+1,\text{LO}}/Z_{n_t,\text{LO}}$$

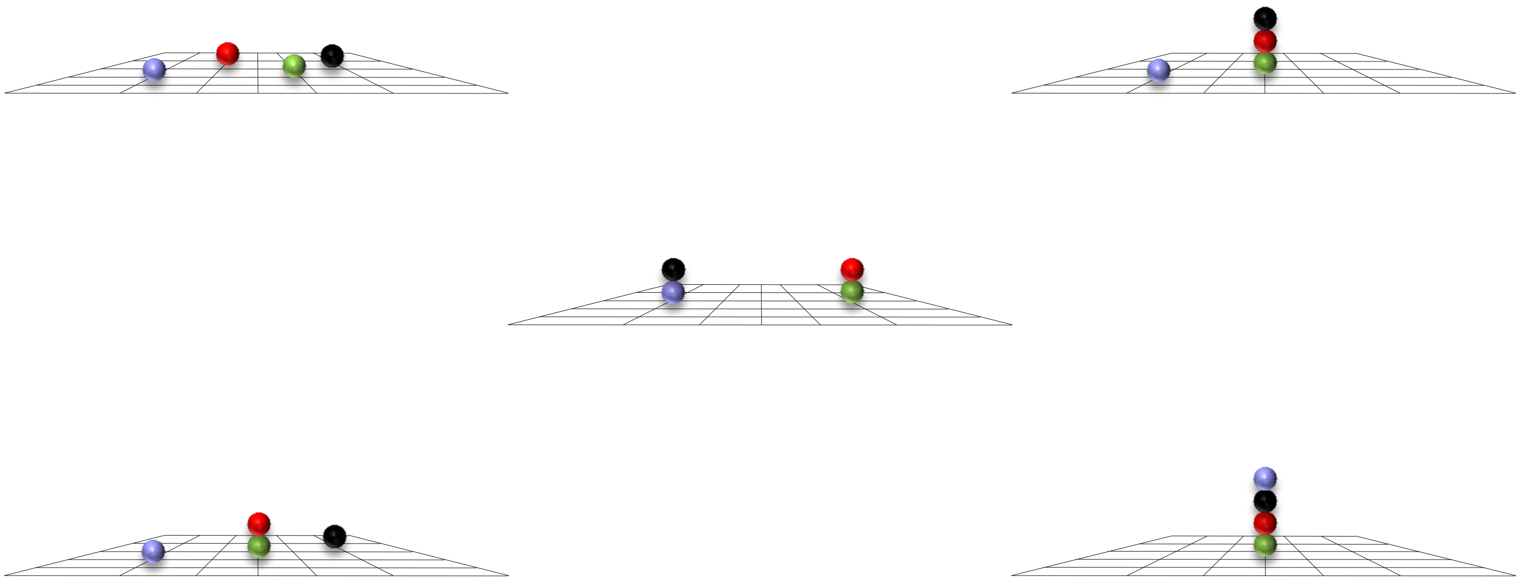
$$\langle O\rangle_{0,\text{LO}} = \lim_{n_t\to\infty} Z^{\langle O\rangle}_{n_t,\text{LO}}/Z_{n_t,\text{LO}}$$

$Z_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

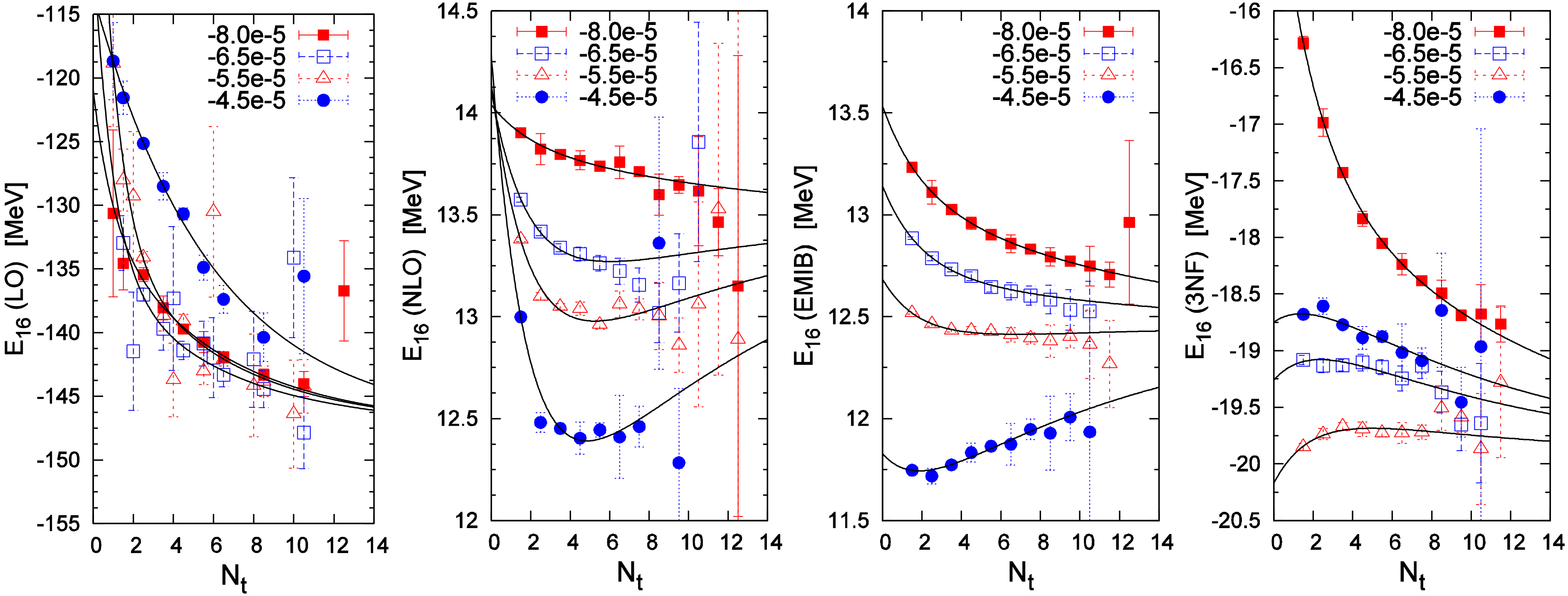
$$\langle O \rangle_{0,\mathrm{NLO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} / Z_{n_t,\mathrm{NLO}}$$

Particle clustering included automatically



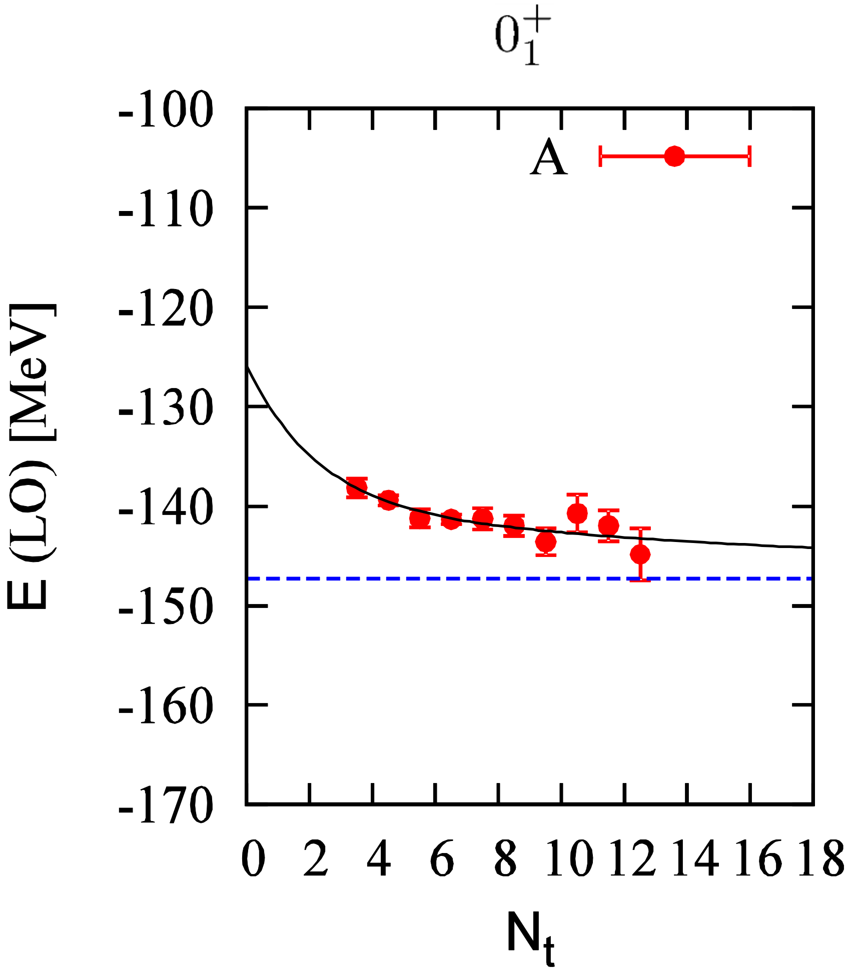
Oxygen-16 ground state

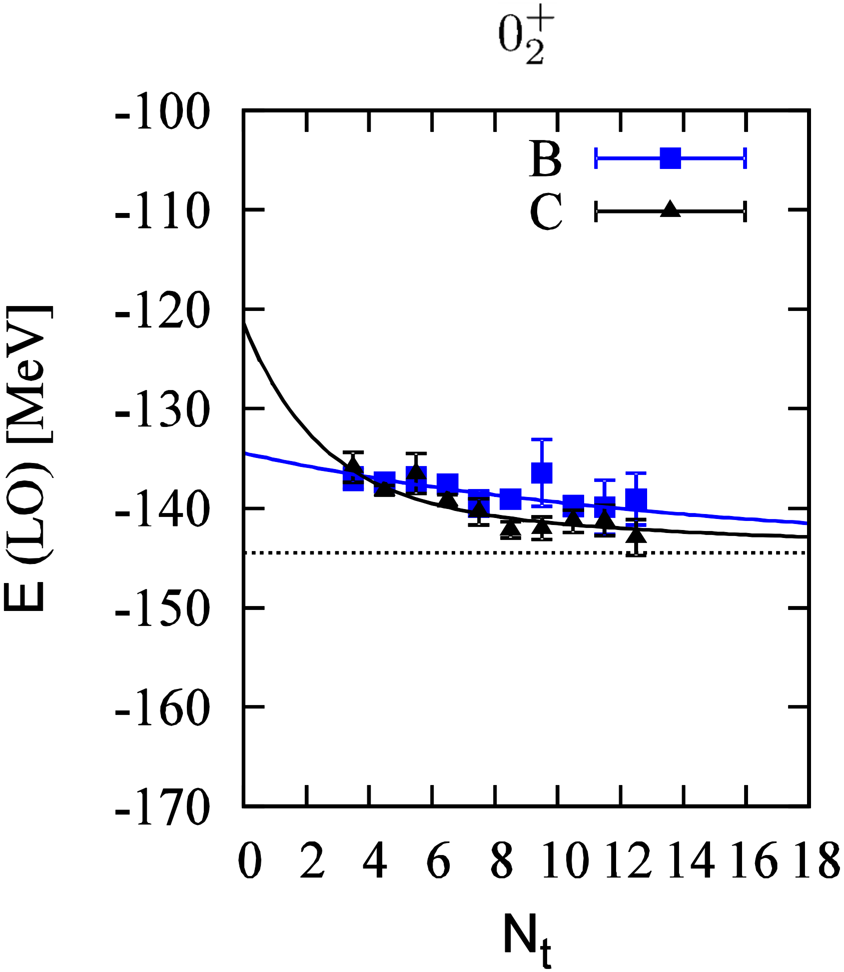
LO NLO EM & IB 3NF



Lähde, Epelbaum, Krebs, D.L, Meißner, arXiv:1311.0477

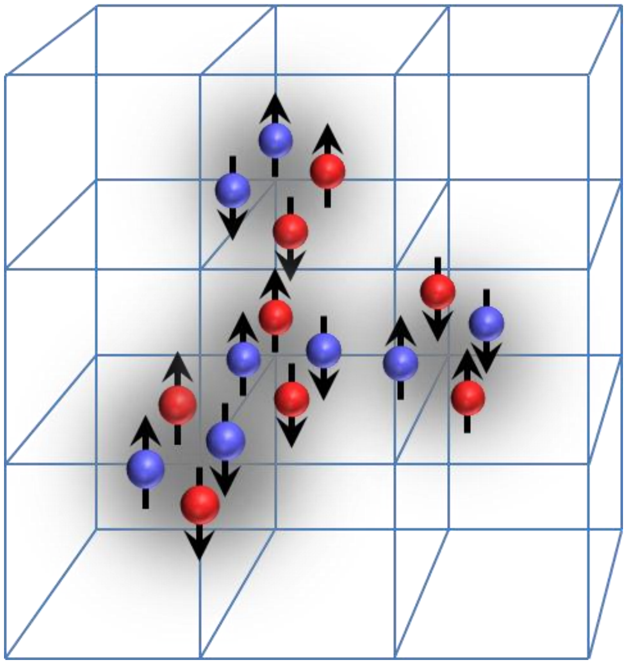
Oxygen-16 spectrum and structure





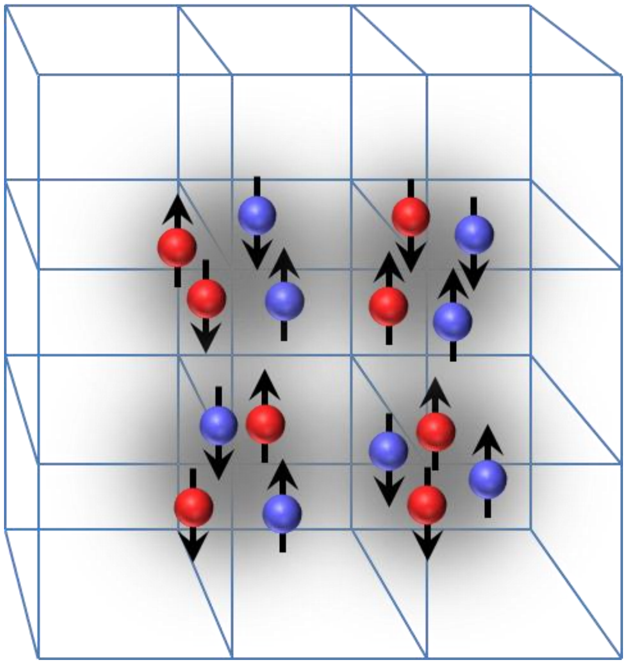
Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1312.7703, PRL in press

0_1^+



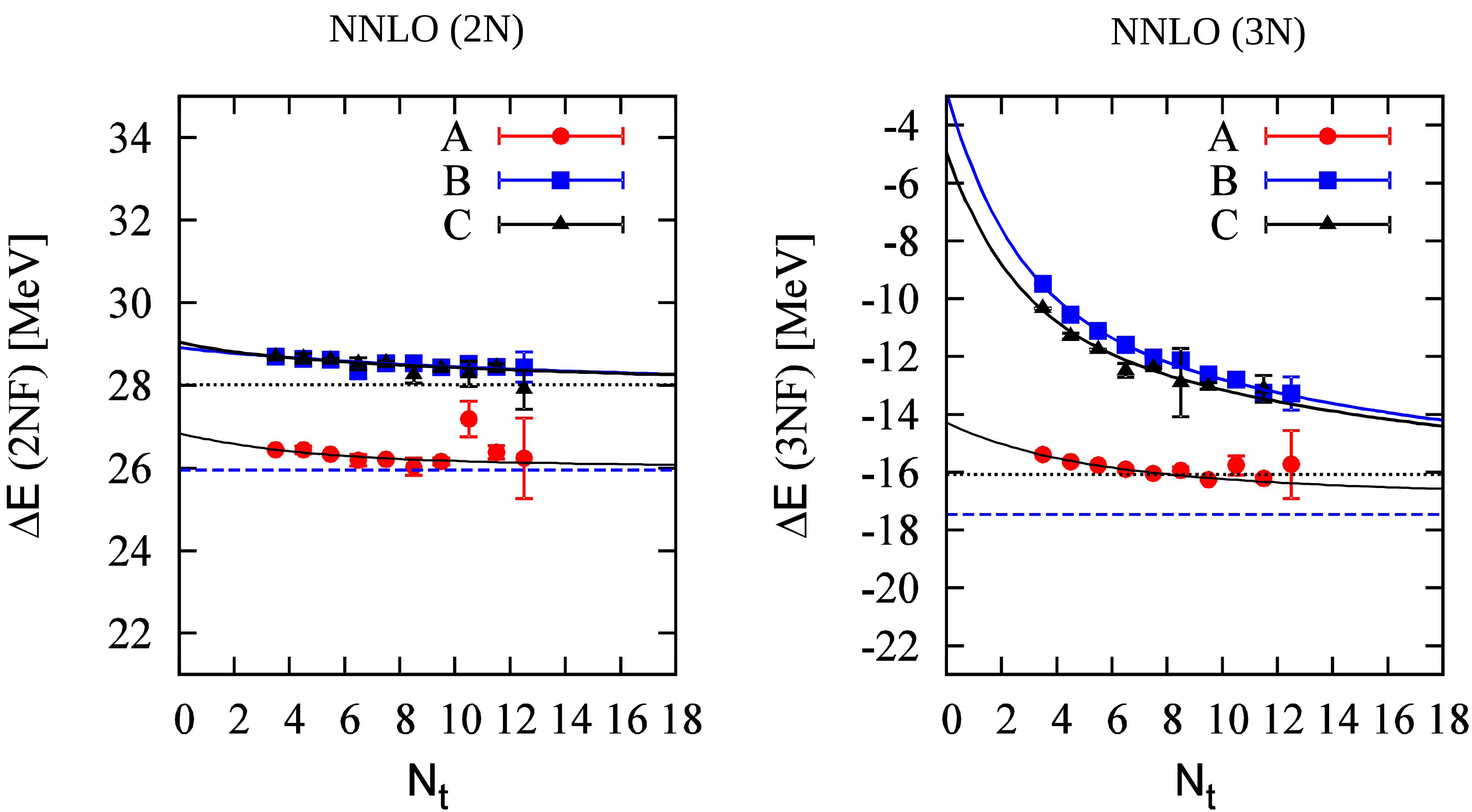
A - Tetrahedral structure

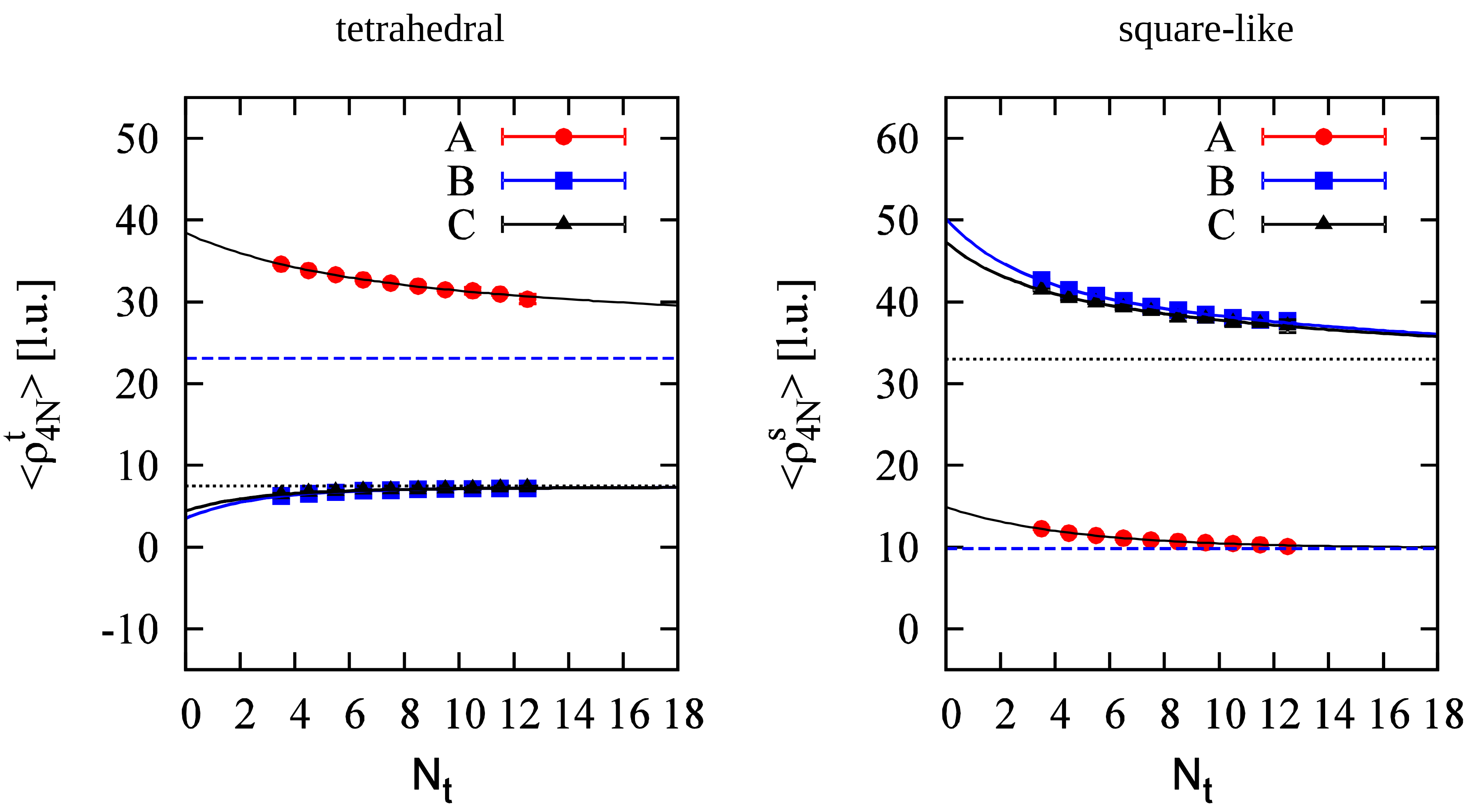
0_2^+



B,C - Square-like structure

Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1312.7703, PRL in press


NNLO (2N)
NNLO (3N)
A
B
C
ΔE (2NF) [MeV]
ΔE (3NF) [MeV]
34
32
30
28
26
24
22
-4
-6
-8
-10
-12
-14
-16
-18
-20
-22
0 2 4 6 8 10 12 14 16 18
N_t



tetrahedral
square-like
A
B
C
$\langle\rho^t_{4N}\rangle$ [l.u.]
$\langle\rho^s_{4N}\rangle$ [l.u.]
N_t

	LO	NNLO (2N)	NNLO (3N)	$+ 4N_{eff}$	Exp.
0_1^+	-147.3(5)	-121.4(5)	-138.8(5)	-131.3(5)	-127.62
0_2^+	-145(2)	-116(2)	-136(2)	-123(2)	-121.57
2_1^+	-145(2)	-116(2)	-136(2)	-123(2)	-120.70

	LO	rescaled	Exp.
$r(0_1^+)[\mathrm{fm}]$	2.3(1)	—	2.710(15)
$r(0_2^+)[\mathrm{fm}]$	2.3(1)	—	—
$r(2_1^+)[\mathrm{fm}]$	2.3(1)	—	—
$Q(2_1^+)[e\mathrm{fm}^2]$	10(2)	15(3)	—
$B(E2, 2_1^+ \to 0_2^+)[e^2\mathrm{fm}^4]$	22(4)	46(8)	65(7)
$B(E2, 2_1^+ \to 0_1^+)[e^2\mathrm{fm}^4]$	3.0(7)	6.2(1.6)	7.4(2)
$M(E0, 0_2^+ \to 0_1^+)[e^2\mathrm{fm}^4]$	2.1(7)	3.0(1.4)	3.6(2)

Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1312.7703, PRL in press

Sign oscillations

$$1 = (2-1)^{1000}$$
$$= 2^{1000} - 1000 \cdot 2^{999} + \frac{1000 \cdot 999}{2} \cdot 2^{998} - \cdots$$

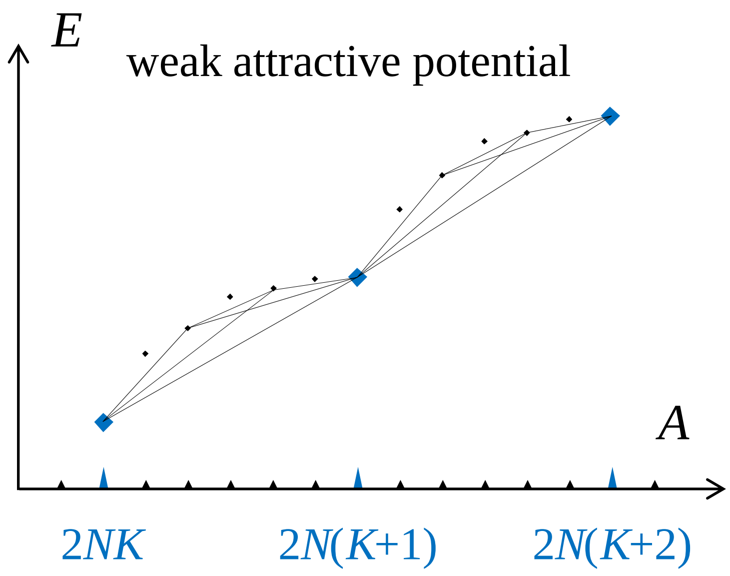
There are different types of sign oscillation problems. In explicit fermion simulations such as diffusion or Green's function Monte Carlo, the sign problem is due to Fermi statistics. In implicit fermion simulations such as auxiliary-field Monte Carlo, the sign problem is predominantly due to repulsive interactions.

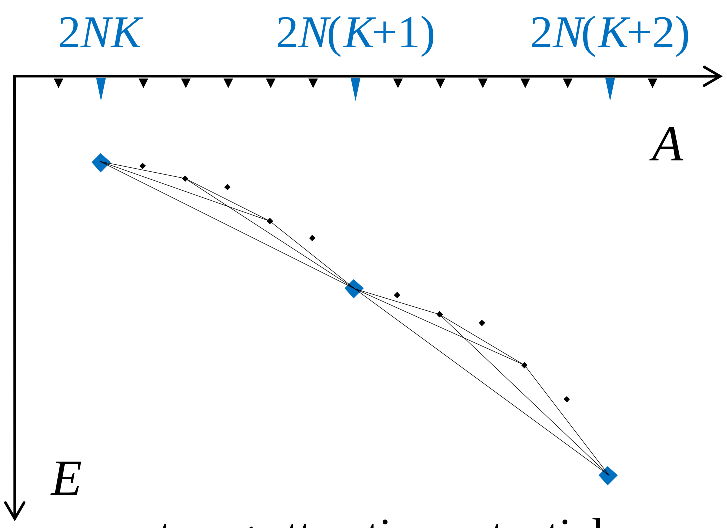
Theorem: Any fermionic theory with SU(2N) symmetry and two-body potential with negative semi-definite Fourier transform obeys SU(2N) convexity bounds.

Corollary: System can be simulated without sign oscillations

Chen, D.L. Schäfer, PRL 93 (2004) 242302;
D.L., PRL 98 (2007) 182501

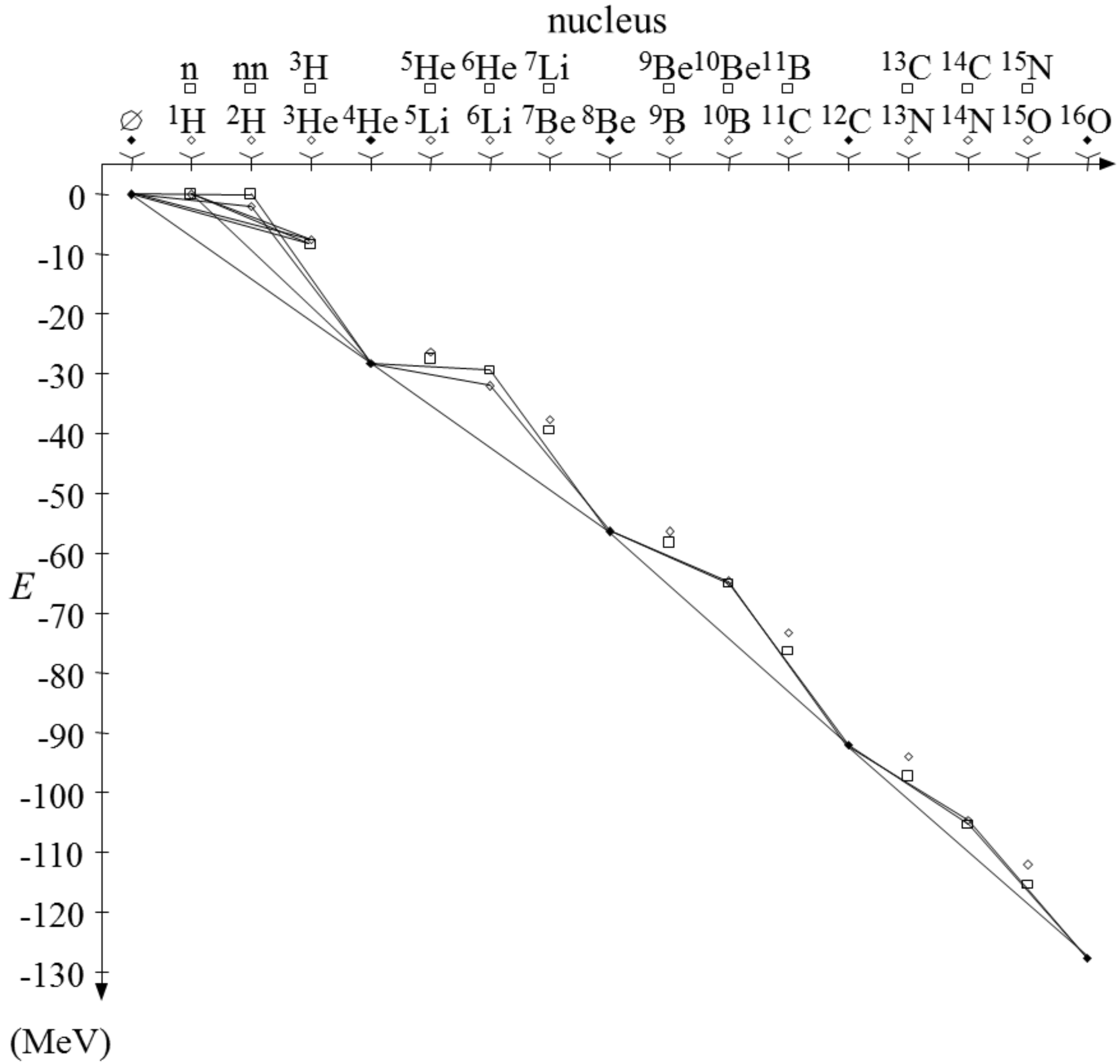
weak attractive potential





strong attractive potential

SU(4) convexity bounds



Symmetry Sign Interpolation Method

Start with a physical Hamiltonian of interest that has a sign oscillation problem

$$H_{\text{phys}}$$

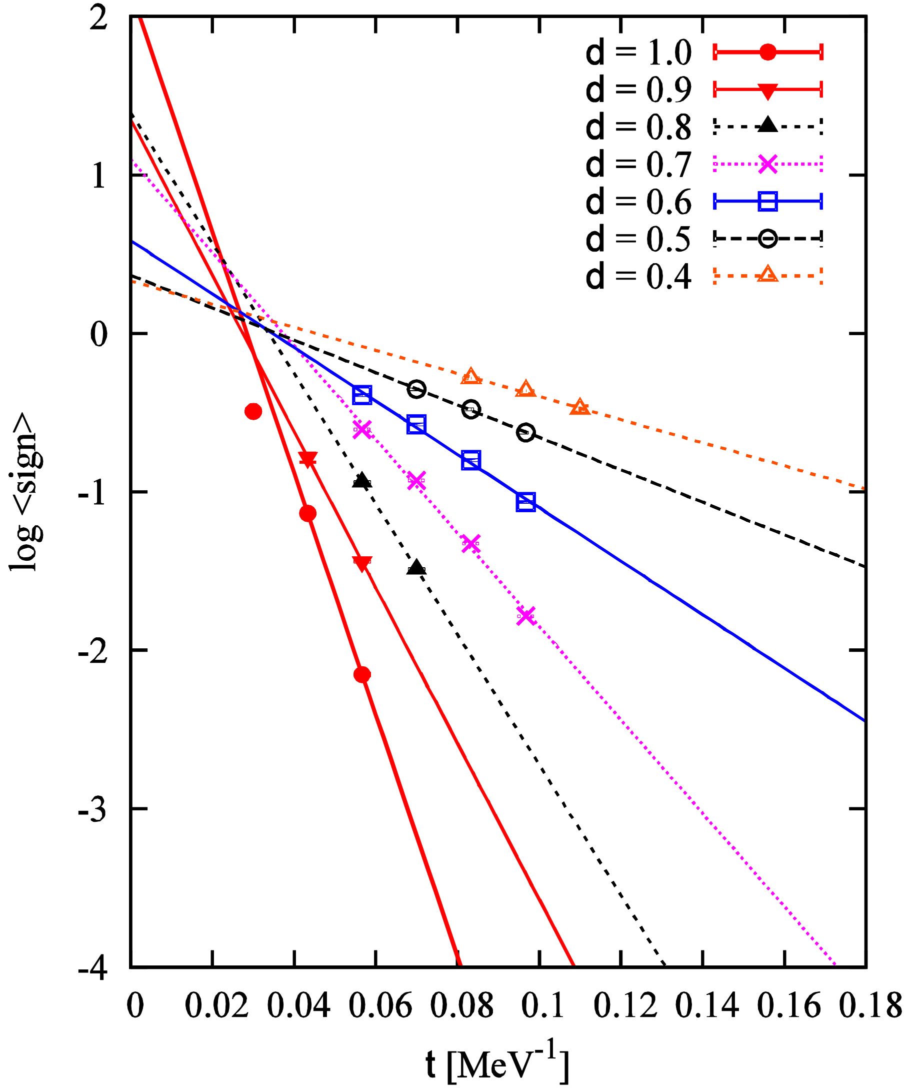
Suppose there exists some SU(2*N*)-invariant Hamiltonian that can be tuned to reproduce the overall size, binding, and other relevant observables for the system of interest

$$H_{\text{SU}(2N)}$$

Construct a one-parameter family interpolating between the two Hamiltonians

$$H_d = (1-d) \cdot H_{\text{SU}(2N)} + d \cdot H_{\text{phys}}$$

$\langle \text{sign} \rangle$



$$\log \langle \text{sign} \rangle \sim -t \cdot d^2$$

$$\langle \text{sign}(H_{\text{phys}}) \rangle \sim 0.01 \Rightarrow \langle \text{sign}(H_{0.7}) \rangle \sim 0.1$$

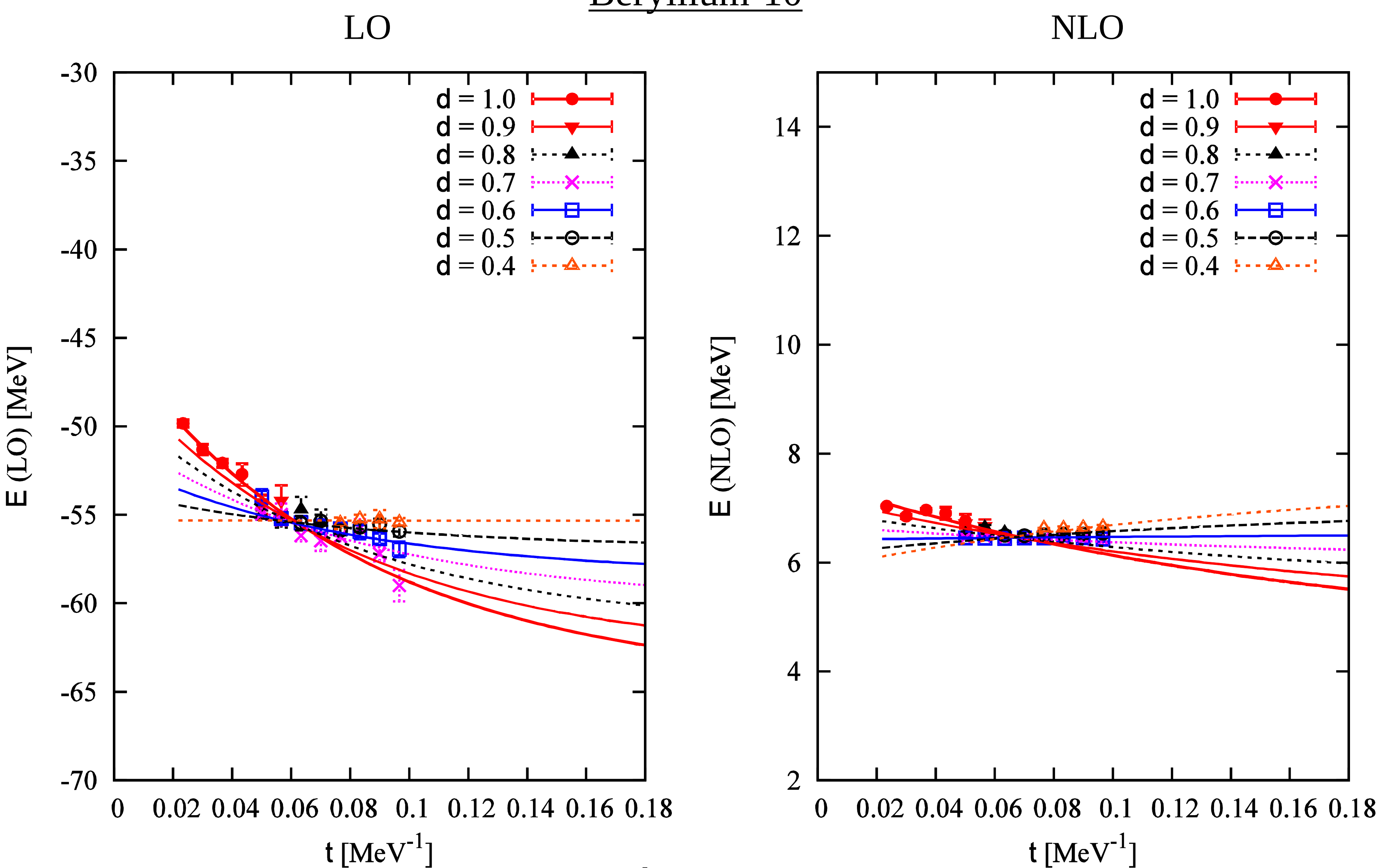
$$\langle \text{sign}(H_{\text{phys}}) \rangle \sim 0.0001 \Rightarrow \langle \text{sign}(H_{0.5}) \rangle \sim 0.1$$

$$\langle \text{sign}(H_{\text{phys}}) \rangle \sim 0.00000001 \Rightarrow \langle \text{sign}(H_{0.35}) \rangle \sim 0.1$$

We now demonstrate the Symmetry Sign Interpolation Method in lattice simulations of the ground state of Beryllium-10. For each energy observable we parameterize the asymptotic dependence of the projected energy as

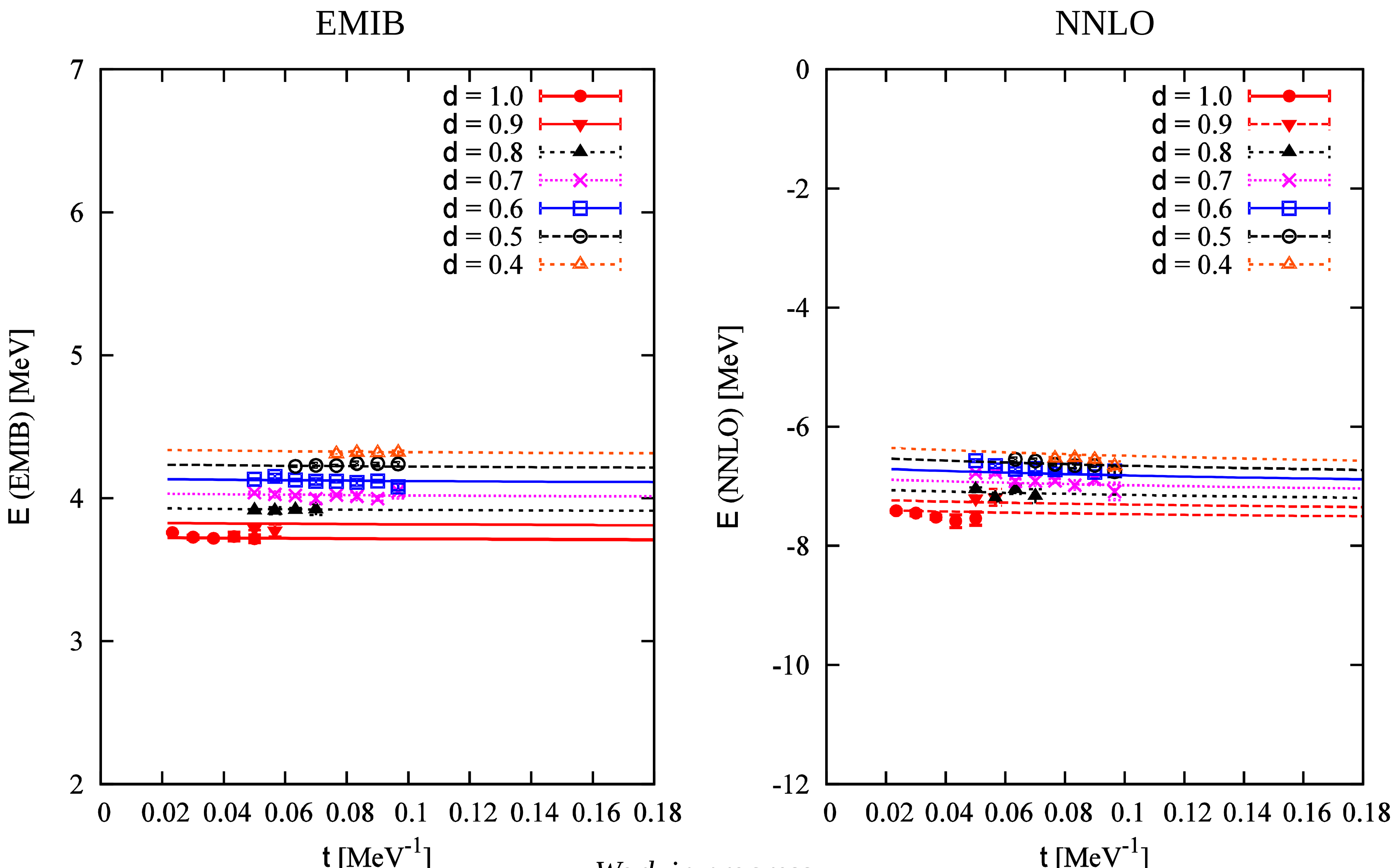
$$E^i(d,t) \to E^i_\infty(d) + c^i(d) \cdot \mathsf{exp}[-\delta E^i(d)t]$$

Beryllium-10



Work in progress

Beryllium-10



Work in progress

Beryllium-10

Preliminary results for ground state energy:

	LO	NLO	NNLO	Exp.
0_1^+	-65(2)	-56(2)	-64(2)	-64.98

includes some NLO terms

Work in progress

Summary

A golden age for nuclear theory from first principles. Big science discoveries being made and many more around the corner.

Lattice effective field theory is a relatively new and promising tool that combines the framework of effective field theory and computational lattice methods. May play a significant role in the future of *ab initio* nuclear theory.

Topics being addressed now and in the near future…

Different lattice spacings, decoupling lattice spacing from ultraviolet regulator, $N \neq Z$ nuclei, elastic and inelastic reactions, neutron matter equation of state and superfluid transition from S-wave to P-wave, etc.